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Topological defects in Spin Density Waves.

N. Kirova and S.Brazovskii.

Laboratoire de Physique Théorique et des Modèles Statistiques, CNRS, Bât.100, Université Paris-Sud, 91405 Orsay cedex, France.
e-mail: kirova@ipno.in2p3.fr brazov@ipno.in2p3.fr

Abstract.
The rich order parameter of Spin Density Waves allows for an unusual object of a complex topological nature: a half-integer dislocation combined with a semi-vortex of the staggered magnetization. It becomes energetically preferable to ordinary dislocation due to enhanced Coulomb interactions in the semiconducting regime. Generation of these objects changes e.g. the narrow band noise frequency.

1 Introduction.

Topological defects in Electronic Crystals - solitons, phase slips (PS) and dislocation lines/loops (DLs) are ultimately necessary for the current conversion and depining processes, see collections [1, 2, 3]. Microscopically in Charge and Spin Density Waves (CDW, SDW, DW) the PS starts as a self-trapping of electrons into solitons with their subsequent aggregation (see [4, 5, 6] for review). Macroscopically the PS develops as the edge DL proliferating/expanding across the sample [8, 7].

An important feature of semiconducting quasi one-dimensional DWs is the Coulomb hardening [9] of their compressibility when the normal carriers freeze out at low temperature T. Then the energetics of DL [10], the accompanying electronic structure [11], etc. are determined by the Coulomb forces limited by screening facilities of remnant free carriers.

The CDW/SDW are characterized by scalar/vector order parameters: $\eta_{cdw} \sim \cos[Qx + \varphi]$, $\vec{\eta}_{sdw} \sim \vec{m} \cos[Qx + \varphi]$ where $\vec{m}$ is the unit vector of the staggered magnetization. Here we will show that SDWs allow for unusual π PSs forbidden in CDWs where only 2π PSs are allowed. Namely in SDW conventional dislocations loose their priority in favor of special topological objects: a half-integer dislocation combined with a semi-vortex of a staggered magnetization vector. Their possible manifestation may be found in a Narrow band Noise (NBN) generation. The π- PSs reduce twice (down to its CDW value $\Omega/j = \pi$) the universal ratio Ω/j of the fundamental NBN

frequency Ω to the mean sliding current j. The splitting of the normal 2π -dislocation to the π ones in energetically favorable due to Coulomb interactions. The magnetic anisotropy confines half-integer DLs in pairs connected by a magnetic domain wall.

Below we first consider the energy of usual DLs in DWs. Then we turn to the special case of SDW and discuss combined topological objects. Finally we discuss various models for the NBN generation and consequences of the existence of combined topological objects in SDW.

2 A single dislocation in semiconducting density wave.

Any stationary configuration is determined by minimization of the energy functional

$$W\{\varphi\} = \int \frac{d\vec{R}}{s} \frac{\hbar v_F}{4\pi} \left[C_\parallel^0 \left(\frac{\partial \varphi}{\partial x} \right)^2 + C_\perp (\nabla_\perp \varphi)^2 \right] + W_C \qquad (1)$$

Here v_F is the Fermi velocity of the parent metal, $\vec{R} = (x, \vec{r})$ with x being the chain direction, $s = a_\perp^2$ is the area per chain. The Coulomb part of the energy, with some simplifications, is

$$W_C = \int d\vec{R}_1 d\vec{R}_2 n_c(\vec{R}_1) n_c(\vec{R}_2) \frac{\exp[-|\vec{R}_1 - d\vec{R}_2|/r_{scr}]}{|\vec{R}_1 - d\vec{R}_2|}\,,\ n_c = \frac{e\rho_c}{\pi s} \frac{\partial \varphi}{\partial x}$$

where n_c is the electric charge density of the locally deformed DW, ρ_c and $\rho_n = 1 - \rho_c$ are the normalized densities of the condensate and of the normal carriers. Recall that $\rho_n \to 1$ at $T \to T_c^0$ and $\rho_n \sim \exp(-\Delta/T)$ at low T being activated through the DW gap 2Δ. The parameters $C_\parallel^0$ and $C_\perp$ are the compression and the share moduli; within our normalization $C_\parallel^0 = \rho_c$ and $C_\perp \sim \rho_c$. In the Fourier representation

$$W\{\varphi\} = \frac{\hbar v_F}{4\pi} \sum |\varphi_k|^2 \left[\rho_c k_\parallel^2 + C_\perp k_\perp^2 + \frac{\rho_c^2 r_0^{-2} k_\parallel^2}{(k_\parallel^2 + k_\perp^2 + r_{scr}^{-2})} \right] \qquad (2)$$

where $r_0 = \sqrt{\hbar v_F s\epsilon/(8e^2)}$ is the screening length in the parent metal and $r_{scr} = r_0/\sqrt{\rho_n}$ is the actual screening length in the DW.

The Coulomb interactions drastically affect the charged phase deformations. They may not be important yet only at shortest interchain distances

$r < r_0$, which are allowed only if $r_0 > a_\perp$, where the usual elastic theory is applicable. Beyond this core but still within the screening distance $r_0 < r < r_{scr}$ we can write the energy, collecting only the senior terms, as

$$W\{\varphi\} \approx \frac{\hbar v_F}{4\pi} \sum |\varphi_k|^2 \left[C_\perp k_\perp^2 + r_0^{-2} \frac{k_\parallel^2}{k_\perp^2} \right] , \; k_\perp \gg r_{scr} \qquad (3)$$

This expression describes a nonanalitic elastic theory with energy dependent on ratio of gradients rather on their values. Finally at large distances $r \gg r_{scr}$ we have

$$W\{\varphi\} \approx \frac{\hbar v_F}{4\pi} \sum |\varphi_k|^2 \left[C_\parallel k_\parallel^2 + C_\perp k_\perp^2 \right] , \; C_\parallel = \rho_c/\rho_n , \; k_\perp \ll r_{scr} \qquad (4)$$

The effective elastic theory is restored but in stretched coordinates $(x\sqrt{C_\perp \rho_n/\rho_c}, r)$. We summarize that the effective compressibility $C_\parallel$ hardens with r (starting from $C_\parallel^0$ at shortest interchain distances) as $C_\parallel \sim r^2/r_0^2$ beyond the screening length of the parent metal $r > r_0 \sim 1\mathring{A}$, until it saturates at r_{scr} at the value which grows activationally with T.

Consider a D-loop of a radius R in the (y, z) plane embracing a number $N = \pi R^2/s$ chains or a D-line stretched in z direction at a distance $Y = a_\perp N$ from its counterpart or from the surface. The DL is characterized by its energy $W(N)$ and by the 'chemical potential' $w = \partial W/\partial N$ which determines the mutual equilibrium among DLs and between them and pairs of normal electrons. The scale of the DL energy per unit length is $E_0/a_\perp$. Within the (effective) elastic theory it is $E_0 \sim \sqrt{C_\parallel C_\perp}\hbar v_F/a_\perp$ where $C_\perp$ is a measure of the interchain coupling. For essentially quasi-1D systems like typical CDWs, where the actual transition temperature $T_c < T_c^0 \sim \Delta$ (so that in the ordered phase always $\rho_c \approx 1$) we have $E_0 \sim T_c$. For systems with wider interchain electronic bandwidth $t_\perp > \Delta$, which is typical for SDWs, the scale is $\tilde{E}_0 \sim \rho_c t_\perp$ which can be larger than $T_c \approx T_c^0$. A characteristic feature of the nonscreened regime (3) is an optimal perpendicular scale $L_\perp = k_\perp^{-1}$ at any given longitudinal scale $L_\parallel = k_\parallel^{-1}$: $L_\perp^2 \sim L_\parallel r_0 C_\perp^{1/2}$. Now multiplying the energy density $\sim C_\perp L_\perp^{-2}$ by the characteristic volume $L_\parallel L_\perp^2$ we estimate the energy as a function of $R = L_\perp$ as $\hbar v_F C_\perp^{1/2} R^2/r_0 = w_C N$ with $N = \pi R^2/r_0$ and $w_C \sim E_0^0 a_\perp/r_0$, $E_0^0 \sim \max[T_c, \rho_c t_\perp]$.

Finally for the D-loop energy $W_D(N)$ one finds [10]:

1. $W_D(N) \sim \sqrt{N} \ln N E_0 \qquad N \sim 1.$
2. $W_D(N) \sim N w_C, w_C \sim E_0^0 a_\perp/r_0 \qquad R < r_{scr} \qquad (N = \pi R^2/s)$
3. $W_D(N) \sim \sqrt{N} \ln N E_0 r_{scr}/r_0 \qquad R > r_{scr}$

For the dislocation energy within r_{scr} there is not a usual perimetric law

$\sim \sqrt{N}$ but rather the area one $\sim N$. At large distances the standard perimetric law is restored but with the greatly enhanced $\sim \rho_n^{-1/2}$ magnitude.

In SDW the energy of a pure magnetic vortex loop $W(\vec{m})$ is not affected by the Coulomb forces, so that its only scale is E_0. We have

$$W_{\vec{m}}\{\vec{m}\} = \int \frac{dxd\vec{r}}{s}\left[\tilde{C}_{\|}\left(\frac{\partial m}{\partial x}\right)^2 + \tilde{C}_{\perp}(\vec{\nabla}_{\perp}\vec{m})^2\right], \qquad W_{\vec{m}}(N) \sim \sqrt{N}\ln N\tilde{E}_0 \tag{5}$$

where $\tilde{C}_{\|}$, $\tilde{C}_{\perp}$ are the elastic moduli related to the rotation of the staggered magnetization unit vector $\vec{m}$. They are similar to phase displacement moduli taken without Coulomb interactions $C_{\|}^0$, $C_{\perp}$, in (1). Hence for the VLs the regime 1. is applicable at all N.

The resulting μ_D of a single D-loop is drown schematically at Fig.1. Here the dashed line corresponds to the magnetic vortex loop. The inner region of the solid line describes both the D-loop and the magnetic vortex.

3 Half-integer dislocation combined with semi-vortex.

In SDWs the Coulomb enhancement of the dislocation energy plays a principal role to bring to life a special combined topological object. This is the half-integer dislocation accompanied by the 180^o rotation $\mathcal{O}_{\pi}$ of the staggered magnetization $\vec{m}$. Indeed, the SDW order parameter $\vec{\eta} = \vec{m}\cos(Qx+\varphi)$ allows for the following three types of self-mapping $\vec{\eta} \to \vec{\eta}$. (The mapping is a general requirement of topological connectivity which selects the allowed configurations [12, 13].)
i. normal dislocation: $\varphi \to \varphi + 2\pi,\ \vec{m} \to \vec{m}$;
ii. normal $\vec{m}$ – vortex: $\vec{m} \to \mathcal{O}_{2\pi}\vec{m},\quad \varphi \to \varphi$;
iii. combined object : $\varphi \to \varphi + \pi,\ \ \vec{m} \to \mathcal{O}_{\pi}\vec{m} = -\vec{m}$.
In the last case both the orientational factor $\vec{m}$ and the translational one $\cos(Qx+\varphi)$ change the sign, but their product $\vec{\eta}$ stays invariant. A necessity of semi-vortices in conventional antiferromagnets in presence of frozen-in host lattice dislocations has been realized already in [14]. In the SDW the semi-vortices become the objects of the lowest energy created in the course of PS process. Indeed only not far below T_c at $\rho_n \sim 1$ the elastic moduli related to the phase displacements and to magnetization rotations are of the same order, hence all three objects have similar energies, $W_D \sim W_{\vec{m}}$. With lowering T the energy of the object ii. is not affected (except for a universal dependence $\sim \rho_c$ near T_c) because charges are not perturbed so that Coulomb forces are not involved. For objects i. and iii. the major energy $\sim \rho_n^{-1/2}$ is associated to distortions of φ so that the energy of $\vec{m}$ rotation in the case iii. may be neglected. To compare main contributions to energies of objects i. and iii. we remind that at given N the DL energy depends on its winding

number ν_φ as $W_D \sim E_0(\rho_s/\rho_n)\nu_\varphi^2$, where $\nu_\varphi = 1/2$ for π-DL and $\nu_\varphi = 1$ for the 2π-DL. The energy of the magnetic vortex depends on the vorticity $\nu_{\vec{m}}$ as $W_{\vec{m}} \sim E_0\rho_s\nu_{\vec{m}}^2$. We must compare their energies at the given number of accumulated electrons $2N$. For shortness consider only the largest (screened) sizes of DLs.

For the D-loop with the radius R and the D-line located at a distance Y from its (spatially image) counterpart we have correspondingly

$N \sim \nu R^2, \qquad \mu_D \sim \partial(\nu_\varphi^2 R \ln R)/\partial(\nu_\varphi R^2) \sim \nu_\varphi^{3/2}/N^{1/2}$

$N \sim \nu Y, \qquad \mu_D \sim \partial(\nu_\varphi^2 \ln Y)/\partial(\nu_\varphi Y) \quad \sim \nu_\varphi^2/N$

In both cases the lowest energy per electron W is given by an object with smallest $\nu_\varphi = 1/2$ i.e. by the combined one, $W = (W_D + W_{\vec{m}})/2 \sim W_D/2$. We conclude that in SDW the normal dislocation must split into two objects of the combined topology with the repulsion between them. Apparently they will have the same sign of the displacive half-integer winding numbers (the total charge $2eN$ must be preserved). But the half-integer spin rotation numbers should have opposite signs (to avoid a divergence of the magnetic energy). In Fig.2 we present the vector field of the local SDW magnetization $\vec{\eta}$ for a single "chimera". The chain axis is horizontal.

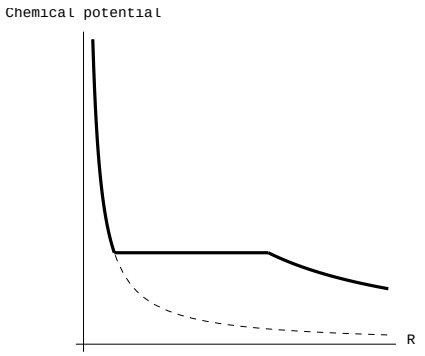

Figure 1: The chemical potential $w = \partial W/\partial N$ of the D-loop. Dashed line corresponds to the model without Coulomb interactions and to the vortex loop.

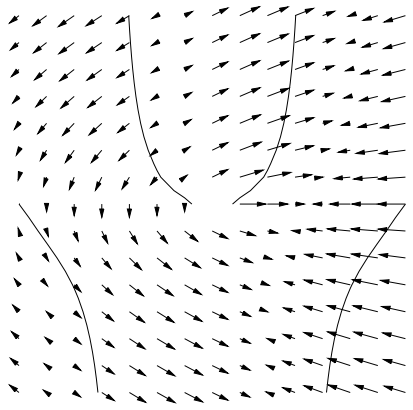

Figure 2: Vector-field $\vec{\eta}$ for half-DL combined with semi-vortex. Solid lines indicate constant phases around the half-DL.

Consider now effects of a *spin anisotropy* which have either spin-orbital or dipole-dipole origin. The "easy plane" case allows for a free rotation of spins, so it will not affect any of above conclusions. The same will hold in case of a pure "easy axis" case but only at presence of magnetic field $H > H_{sf}$ exceeding the spin-flop field $H_{sf} \sim 1T$ above which the spins will be tilted thus possessing a free rotation at the hard plane. But the known SDW crystals have low symmetry, which originates the spin anisotropy in all three

directions. Being small, the anisotropy will not affect the arrangement in a vicinity of the DL where the gradient and the Coulomb energies dominate. But at large distances from the DL the free rotation of spins is prohibited. The π-rotation of spins will be concentrated in space within the Neél domain wall. It will form a string (a plane in 3D) which confines the two combined objects. Indeed at $r < r_{scr}$ the total energy gain with respect to the normal DL is $-E_C N/2$ while the energy lost due to domain wall formation is $W^A_{\vec{m}} = w^A N$, thus both having a similar N dependence. Usually $w^A \sim 1K/chain < E_C$ and we have a constant repulsion between the two chimeras. But beyond the screening volume $r > r_{scr}$ the total energy gain of two objects with respect to one DL is $W = -(E_0/\sqrt{\rho_n}) \ln N + w^A N$ - the Coulomb energy slows down while the $W^A_{\vec{m}}$ keeps growing linearly. Hence there is an equilibrium distance between the chimeras $N_{eq} \sim E_0/(w^A\sqrt{\rho_n})$. The confined objects can be shown to split off along the interchain direction. Usually the spin anisotropy is noticeable only for one orientation and characterized by the spin-flop field $H_{s-f} \sim 1T$. It would originate the string of the length $\sim 0.1\mu m$. At higher magnetic fields only a small in-plane anisotropy is left so that the string length may reach the sample width which is typically $\sim 1\mu m$.

4 Combined topological defects and the NBN generation.

The DWs generate the Narrow Band Noise which is a coherent periodic unharmonic signal with the fundamental frequency Ω being proportional to the mean *dc* sliding current j with the universal ratio Ω/j [15]. In CDW ideally $\Omega/j = \pi$ which corresponds to carrying of two electrons by displacing of the CDW by its wave length λ. In SDW the ratio has been accessed only indirectly [16, 17] with the different experiments being in favor of either the $\Omega/j = \pi$ of the twice higher ratio $\Omega/j = 2\pi$. Surprisingly the origin of such a bright effect as the NBN has not been identified yet with main pictures competing:
The Wash-Board Frequency (WBF) model suggests that the NBN is generated extrinsically while the DW modulated charge passes through the host lattice sites or its defects [18].
The Phase Slip Generation (PSG) model suggests that the NBN is generated by the phase discontinuities occurring near injecting contacts [8, 7]. Recall that CDW and SDW order parameters are

$$\eta_{cdw} \sim \cos[Qx + \varphi] \text{ and } \vec{\eta}_{sdw} \sim \vec{m}\cos[Qx + \varphi]$$

where $\vec{m}$ is the vector of the staggered magnetization. Importantly the oscillating densities are

$$\rho_{cdw} \sim \eta_{cdw} \sim \cos[Qx + \varphi], \text{ but } \rho_{sdw} \sim \delta(\vec{\eta}_{cdw})^2 \sim \cos[2Qx + 2\varphi]$$

So the SDW charge modulation wave length is only half of the CDW one $\lambda = 2\pi/Q$. Hence within the WBF model the NBN frequency Ω is doubled: In CDW $\Omega = -\dot{\varphi} = \pi j$ while in SDW $\Omega = -2\dot{\varphi} = 2\pi j$.

At first sight the observation of the twice different ratios is natural from the point of view of the WBF model. Nevertheless the WBF model has an unresolved weaknesses. The original concept implied the interaction between the rigid DW and the regular host lattice $\sim \cos(n\varphi)$ where the commensurability index is typically $n = 4$ which would give an n- fold WBF contrary to experiments. Nowadays a common belief is that the necessary potential $V_{imp} \sim \cos\varphi$ is provided by the host impurities. But actually $V_{imp} \sim \cos(Qx_i + \varphi)$ so that the positionally random phase shifts $\sim Qx_i$ will prevent any coherence in linear response. (The mode locking (Shapiro steps) is still possible as a second order nonlinear effect.) But for the linear effects the only possibility left is to suppose that the DW does not slide at the sample surface so that the coupling $\sim \cos(\varphi_{bulk} - \varphi_{surface})$ would provide a necessary WBF.

The PSG model (see [7] and refs. in [11, 19]) is attractive because the PSs are ultimately necessary to provide the current conversion at the contacts. A weak point of the PSG model is to explain their regularity: e.g. only one DL can flash across at a given time while the next DW is waiting for the next DW period to pass. The topological connectivity requires that after the phase slip or going around the dislocation the order parameter should be mapped onto itself. For crystals it means that exactly one lattice period enters or in terms of dislocation language one says that the dislocation Burgers vector coincides with the lattice period, which is 2π in x - direction in our case. Since the unit sells of the CDW and the SDW are the same (2 electrons) the $\Omega/j = \pi$ would be the same, which contradicts to the latest experimental results [17]. This argument has been used to exclude the PSG mechanism in favor to the WBF one. A generation of half-integer DLs resolves this contradiction by twice increase of Ω/j. These "chimeras" are energetically favorable at low temperatures, when the number of free carriers is small. But near the SDW transition temperature the energies of a magnetic vortex and of a the dislocation are comparable. Then the possibility of usual DL to split into two combined objects depends on the material parameters. It means that for SDW near T_c the ratio Ω/j in not universal. For some materials it can be 2π in the whole temperature range if the splitting of dislocation is energetically favorable already near T_c, for other materials the ratio Ω/j can change from $\Omega/j = \pi$ at high temperatures to $\Omega/j = 2\pi$ at low temperatures passing through the region of intermediate values when both simple dislocations and "chimeras" coexist. Notice also a necessity of studying the narrow sample which is indeed the case for molecular crystal with SDWs. Otherwise the string length created by the spin anisotropy will be shorter than the sample width and the chimers will propagate in loosely bound pairs.

5 Conclusions.

We conclude that the sliding SDW should generate "chimers": the combined topological objects where the spin rotations are coupled to the DW displacements. They are stable by lowering the DL Coulomb energy. This combination effectively reduces the SDW period allowing e.g. for the twice increase in the NBN frequency, which is an important disputable question. The interest in such unusual topological objects may go far beyond the NBN generation or the current conversion problem in SDWs. Actually the studies on these complex patterns would correlate to current interest in formation of topological objects from superfluid ^3He to the model of earlier Universe [20].

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